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# FORMULATION AND PROCEDURE TO TREAT A DISCRETE PARTICLE MODEL AS A CONTINUUM

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## 1 INTRODUCTION

This paper continues the path opened by previously published researches related to numerical models and stress-strain behaviour discrete particle models [1], [2] and [3].

In those researches was enounced how to generate numerically a granular media, assimilating the particles to spheres and adjusting the probability of appearance of a given size according to a grain size distribution.

Afterwards, the behaviour of these generated medias was set out as stiffness matrixes systems using a non-linear law of behaviour (Hertz´s Law) and allowing the particles to slide in their relative rotations according to Coulomb´s Law. Solving the system in these conditions displacements and forces were calculated for every contact in the media. This calculus is repeated for an increasingly external load. However, this huge amount of information must be treated somehow.

This paper presents a way to solve the problem of the great quantity of information obtained from the calculi, showing a methodology to transform all this discrete particle model information into an equivalent continuum.

## 2 COSSERAT´S DISCRETE MEDIAS

### 2.1 Introduction

The mechanical behavior of a body B formed by three dimension discrete particles X is going to be studied. These particles are a numerable set that interact one with each other. The particles are considered to be semi-rigid. This means that the particle´s deformation only occurs locally in the contact for effect of forces and does not deform in the rest of the particle.

The particles of this study are spheres whose radius adjust to a grain size distribution being the probability of appearance of a certain dimension, directly proportional to the quantity of retained material in that dimension.

The defined body (B) has mass, m(B). This mass is a scalar quantity and is always positive. In addition, the mass can be sum for two bodies, $B_1$ and $B_2$:

$$m(B_1 + B_2) = m(B_1) + m(B_2) \quad (1)$$

The body B has internal structure; this means that every particle of the body has attached axis in a certain orientation to identify the displacements and the rotations. A Scheme of these axis are shown in Figure 1. Due to the attached axis every particle has a momentum $I^{\alpha}$, because the particles are spherically shaped, the momentums around the three axes are the same and equal to $(2/5)\cdot M\cdot R^2$.

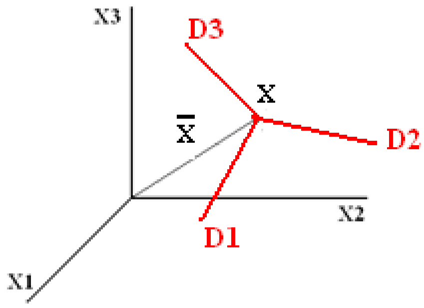


Figure 1.- Scheme of global axis {X1, X2, X3} and local axis {D1, D2, D3}.

The particles X that formed up the body B occupy a place in space at a certain time. The space is Euclidean, this allow choosing a rectangular Cartesian coordinate system once and for all. This is what is called the Common Reference System (CRS). In addition, space has vector structure.

The particles X can be referred to the CRS by a position vector $\bar{X}$ attached to the gravity center and orientated according to the position of the axis previously defined in a certain direction $D^{\alpha}$. Figure 1 shows a scheme of the position vector and the orientation of the axis.

Time is a scalar and both an absolute and relative time exists. The relative time is referred to a time, t=0, choose once and for all. The initial time, t=0, constitute a reference analogous as the CRS is reference of the position in space.

### 2.2 The movement

The place $\bar{X}$, occupied by the particles X in a certain time $t$ and the orientation of those particles, $D^{\alpha}$, is called configuration in time $t$ of the body B. For an instant $t$, every particle has a position $\bar{X}$ and an orientation $D^{\alpha}$.

$$\bar{X} = \bar{X}(X,t) \tag{2}$$
$$D^{\alpha} = D^{\alpha}(X,t) \tag{3}$$

During time a particle X acquires different positions $\bar{x}$ and different orientations $d^{\alpha}$. The evolution of these variables are called movement laws and specifies the position and orientations of a given particle:

$$\bar{x} = \bar{x}(X,t) \tag{4}$$
$$d^{\propto} = d^{\propto}(X,t) \tag{5}$$

The movement laws can be then expressed:

$$\bar{x} = \bar{x}(\bar{X},t) \tag{6}$$
$$d^{\propto} = d^{\propto}(\bar{X},t) \tag{7}$$

### 2.3 Displacements and rotations

A particle has 6 grades of freedom; three of them are related to the displacements; and the other three to the rotations. The displacements ($u$) are calculated by subtracting the position vector $\bar{x}$ in the time $t$ against the position $\overline{X_0}$ in the time t=0.

$$\bar{u} = \bar{x}(\bar{X},t) - \bar{X}_0 \tag{8}$$

The rotations correspond to the axial vector $\bar{\phi}$, which is the rotation that carries de axis $D^{\alpha}$ from their initial positions to their final position $d^{\alpha}$ in time $t$. The axial vector $\phi$ is equivalent to a hemi-symmetric rotation tensor w:

$$\bar{w} = -\bar{\varepsilon} \cdot \bar{\phi} \tag{9}$$

Where; $\bar{\varepsilon}$ is Ricci´s permutation tensor of third order.

The rotation tensor $R^c$ of Cosserat is the one that carries the axis from $D^{\alpha}$ to $d^{\alpha}$, being:

$$d^{\alpha} = R^c \cdot D^{\alpha} \tag{10}$$

Where; $R^c = \exp(\bar{w})$. For small movements can be said that:

$$R^c = \bar{I} - \bar{\varepsilon} \cdot \bar{\phi} \tag{11}$$

$\bar{I}$ is the identity tensor. Then:

$$d^{\alpha} = (\bar{I} - \bar{\varepsilon} \cdot \bar{\phi}) D^{\alpha} \tag{12}$$

Operating, an analogous expression to the one of the displacement is obtained but referred to the rotations:

$$d^{\alpha} - D^{\alpha} = -\bar{\varepsilon} \cdot \bar{\phi} \cdot D^{\alpha} \tag{13}$$

## 3 INTERACTIONS

In this point is studied the mobilized forces and the geometry of a contact between two particles after a displacement ($\bar{u}$) takes places. A particle *1*, exerts over a particle *0* some actions that generates a normal and shear force $\mathcal{F}$ that in local axis components can be expressed as the summation of; $\mathcal{F}_N^{01}$; $\mathcal{F}_{T1}^{01}$; *and* $\mathcal{F}_{T2}^{01}$ and in addition produces a torque $\mathcal{M}$ that in the same local axis can be decomposed in; $\mathcal{M}_T^{01}$; $\mathcal{M}_{F1}^{01}$; *and* $\mathcal{M}_{F2}^{01}$. The forces mobilized in a contact are shown in Figure 3.

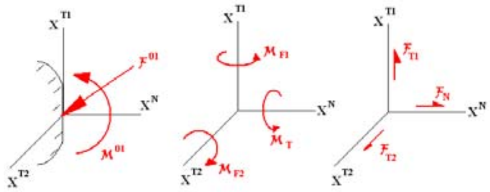

Figure 3.- Mobilized forces and torques in a contact.

For a certain differential variation of the relative movements between the particle 1 and the particle 0, the following actions are analyzed:

$$d\mathcal{F} = \begin{bmatrix} d\mathcal{F}_N \\ d\mathcal{F}_{T1} \\ d\mathcal{F}_{T2} \end{bmatrix} \quad \text{and} \quad d\mathcal{M} = \begin{bmatrix} d\mathcal{M}_T \\ d\mathcal{M}_{F1} \\ d\mathcal{M}_{F2} \end{bmatrix} \qquad \text{(14) and (15)}$$

These forces appear due to the differential movements:

$$du^0 = \begin{bmatrix} du^0{}_N \\ du^0{}_{T1} \\ du^0{}_{T2} \end{bmatrix} \;;\; du^1 = \begin{bmatrix} du^1{}_T \\ du^1{}_{F1} \\ du^1{}_{F2} \end{bmatrix};\; d\phi^0 = \begin{bmatrix} d\phi^0{}_N \\ d\phi^0{}_{T1} \\ d\phi^0{}_{T2} \end{bmatrix} \quad \text{and} \quad d\phi^1 = \begin{bmatrix} d\phi^1{}_T \\ d\phi^1{}_{F1} \\ d\phi^1{}_{F2} \end{bmatrix} \tag{16}$$

The following relations are verified:

$$d\mathcal{F} = K^F \cdot du^{R*} \tag{17}$$

$$d\mathcal{M} = K^M \cdot d\phi^R \tag{18}$$

Where:

$$du^{R*} = du^{1*} - du^{0*} \tag{19}$$

$$du^* = du + r \wedge d\phi \tag{20}$$

$$d\phi^R = d\phi^1 - d\phi^0 \tag{21}$$

$$K^F = \begin{bmatrix} K_N^F & 0 & 0 \\ 0 & K_T^F & 0 \\ 0 & 0 & K_T^F \end{bmatrix} \quad and \quad K^M = \begin{bmatrix} K_T^M & 0 & 0 \\ 0 & K_F^M & 0 \\ 0 & 0 & K_F^M \end{bmatrix} \qquad \text{(22) and (23)}$$

Two different types of materials can be considered:

- Non welded: where do not exist a cohesive material joining the particles.
- Welded: where a cohesive material joins the particles.

For a non welded material the value of $K_N^F$ can be defined by Hertz´s contact Law:

$$K_N^F = \frac{E}{1-\upsilon^2}\sqrt{\frac{r_1 r_2}{r_1+r_2}(u_N^1 - u_N^2)} \tag{24}$$

$$d\mathcal{F}^N = K_N^F \cdot du^N \tag{25}$$

Where; $r_1$ and $r_2$ are the radius of the particles in contact; E is Young´s modulus of the material of the particles; ν is Poisson´s ratios of the particle´s material; and $u_N^1 - u_N^2$ is the total relative displacement of one particle against the other.

$K_T^F$ can be calculated as a portion of the normal stiffness using:

$$K_T^F = \alpha \cdot K_N^F \tag{26}$$

Where α is a coefficient that usually takes the value of 1/3.

The torque tensor can be equaled to zero because only friction can be mobilized in the contact, that is why $K_T^M$ and $K_F^M$ are zero. But in the future and with a research that could guarantee the results could be possible to have very slight values for $K_T^M$ and $K_F^M$ representing that small torques could be possible to be mobilized.

While for a welded material, particles are joined together by a cohesive material as shown in Figure 5. The stiffness coefficients are obtained using numerical methods and modelling, considering the joining material as an elastic cylinder of radius *a* and *h* height. That is to say, the stiffness coefficients are function of the ratio h/a; E and ν. Knowing these coefficients, the forces and torques can be expressed as follow:

$$d\mathcal{F}^N = K_N^F \cdot du^N \tag{27}$$

$$d\mathcal{F}^T = K_T^F \cdot du^T \tag{28}$$

$$d\mathcal{M}^T = K_T^N \cdot d\phi^T \tag{29}$$

$$d\mathcal{M}^F = K_F^M \cdot d\phi^F \tag{30}$$

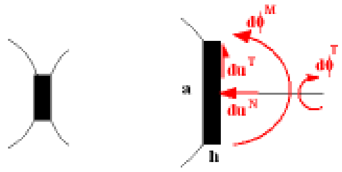


Figure 5.- Scheme of a welded material contact.

## 4 PROPOSAL OF FORMULATION

### 4.1 Introduction

In this point is presented the proposal of formulation that can be used to treat a discrete particle model as a continuum by analyzing the media as a set of particles and as a set of particles forming a continuous material. The final results of all this method will be the stress tensor; the deformation tensor; the torque tensor and the curvature tensor.

### 4.2 Strain formulation

In order to calculate the equivalent strain tensor of the discrete particle model is necessary to consider two situations in different times, as was stated in the previous point. However, the calculi done with the model is not time dependent but loading dependent instead. This is why the time in this formulation is substituted by the value of the external load. In this way and for a predetermined configuration, a particle will be defined by its position vector $\overline{\boldsymbol{X}}$ for a given load and by its new position vector $\overline{\boldsymbol{x}}$ after having increased the external load.

If the movements of every particle are studied between one loading step and another, a displacement gradient ($F_{ij}$ is the displacement gradient tensor) and a rotation gradient ($K_{ij}$ is the curvature tensor) can be defined as follows:

$$\bar{F} = \frac{\partial \bar{x}}{\partial \bar{X}} \tag{31}$$

$$F_{ij} = \frac{\partial x_i}{\partial X_j} = x_{i,j} \tag{32}$$

$$\bar{K} = \frac{\partial \bar{\varphi}}{\partial \bar{X}} \tag{33}$$

$$K_{ij} = \frac{\partial \varphi_i}{\partial X_j} = \varphi_{i,j} \tag{34}$$

However, the movement of a particle is conditioned by all the particles that surround it. In addition, the particle does not suffer a deformation itself, although the deformation that has interest for us is the one of the media. That is why to apply this formulation is necessary to establish a set of particles to which this methodology will be applied. These set of particles are called the contour particles.

All the mechanics concepts that will be expressed from now on are referred to a certain particle of center P. This particle should be as near as possible to the center of the media in order to not being affected by the boundary conditions.

- A fictitious sphere of radius R and center P is defined.

- The particles of the granular media will be in one of the following sets related to the fictitious sphere:

1) Set of inside particles (I); this set is formed by all the particles inside the fictitious sphere.

2) Set of contour particles (C); this set is formed by all the particles that are intersected by the fictitious sphere, that is to say, is formed by every sphere which surface has a part inside the sphere and the other part out of it.

3) Set of exterior particles (E); this set is formed by all the particles that has no contact with the fictitious sphere and not belong to the set of inside particles.

The joint of particles that belong to I and C sets constitute a macro element of radius R inside the discrete media. The contacts of the exterior particles with the contour particles are called effective contacts. That is to say, an effective contact is a contact that belongs simultaneously to the set E and C.

Using (32) the displacement gradient tensor can be expressed as:

$$F_{ij} \cdot dX_j = dx_i \tag{35}$$

The gradient $F_{ij}$ is the displacement gradient of a particle $i$ respect the axis $j$, being the axis centered in the particle P. That is to say, this gradient represent the variation of the relative movement of the particle $i$ respect the particle P, for two different loading values. Figure 6 shows a scheme of this situation, where; P is the center particle, 1,2 and 3 are the centers of particles of the media and belonging to the set C.

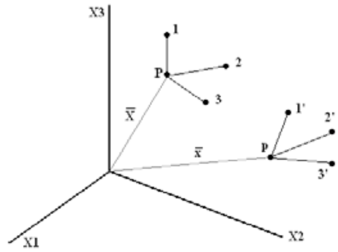


Figure 6.- Scheme of the situation of the contour particles between two different loading steps and their relative displacements.

In the other hand, the curvature tensor can be written:

$$K_{ij} dX_j = d\varphi_i \tag{36}$$

Considering the tensor $F_{ij}$ as the unknown factor and the particle displacements as known (for being the result of the model calculus), an error function can be defined as the difference between the theoretical displacement of a particle ($d\bar{x}^{k*}$) and the real displacement ($d\bar{x}^{k}$) using the global strain tensor.

$$\bar{E}_r = d\bar{\boldsymbol{x}}^{k*} - d\bar{\boldsymbol{x}}^{k} \tag{37}$$

To obtain the displacement gradient tensor the modulus of the error must be minimized. The error of a particle $k$ will be written as follow:

$$\|E_r^k\| = \sum_i \left(F_{ij} dX_j - dx_i\right)^2 \tag{38}$$

The error of all the particles of the set C will be expressed as:

$$E = \sum_k E_r^k = \sum_k \left(\sum_{i=1}^{3} \left(F_{ij} dX_j - dx_i\right)^2\right) \tag{39}$$

In order to minimize the error is necessary to derivate respect the displacement gradient tensor:

$$\frac{dE}{dF_{ij}} = 0 \tag{40}$$

$$\frac{dE}{dF_{ij}} = 2 \sum_i \left(F_{ij} dX_j - dx_i\right) dX_s = 0 \tag{41}$$

$$F_{ij}\left(\sum \quad dX_j dX_s\right) - \left(\sum \quad dx_i dX_s\right) = 0 \tag{42}$$

The following system of equations is obtained after having operated the minimizing procedure:

$$F_{ij}A_{js}{}^{F} = H_{is}{}^{F} \tag{43}$$

Where:

$F_{ij}$ is the displacement gradient tensor.

$A_{js}{}^{F} = \sum \ dX_j dX_s$ The summation index covers every particle of the contour.

$H_{is}{}^{F} = \sum \ dx_i dX_s$ The summation index covers every particle of the contour.

The unknown factor is $F_{ij}$ and it can be finally obtained:

$$F_{ij} = H_{is}{}^{F} A_{js}^{-1\,F} \tag{44}$$

Similarly as has been done with the displacement gradient tensor, the process can be repeated to obtain the curvature tensor $K_{ij}$ rewriting the expressions (37) to (42) in terms of rotations instead of displacements using (36). The curvature tensor can be written:

$$K_{ij}A_{js}{}^{K} = H_{is}{}^{K} \tag{45}$$

Where:

$K_{ij}$ is the curvature tensor.

$A_{js}{}^{K} = \sum \ dX_j dX_s$ The summation index covers every particle of the contour.

$H_{is}{}^{K} = \sum \ d\varphi_i dX_s$ The summation index covers every particle of the contour.

Clearing from (45) $K_{ij}$ is obtained:

$$K_{ij} = H_{is}{}^{K} A_{js}^{-1\,K} \tag{46}$$

In the other hand, if the stretch of an element is considered as the difference between the modulus of the distances, ($ds^2$-$dS^2$) and according to (31) and (32) it can be said that:

$$ds^2 - dS^2 = [F_{KM}^{T} F_{KM} - \delta_{KM}] dX^M dX^K \tag{47}$$

The deformation can be expressed:

$$2E = F^T \cdot F - I \tag{48}$$

Where; E is the Green-Saint Venant deformation tensor; I is the identity tensor and F is the displacement gradient tensor defined in (44).

The deformation tensor (E) can be written in terms of the Cauchy-Green tensor [5]:

$$C = F^T \cdot F \tag{49}$$

$$2E = C - I \tag{50}$$

Where; F is the displacement gradient tensor defined in (44); and C is the Cauchy-Green tensor.

In order to obtain the deformation tensor of the media the following process is proposed:

1) Select a particle inside the media under a certain loading, avoiding choosing a particle near the boundaries. This particle will be P.

2) Generate a fictitious sphere of radious R. By doing this a set of contour particles will be defined (see Figure 4). These contour particles are the ones that are intersected by the fictitious sphere.

3) For every particle “m” belonging to the contour, its displacements and rotations are known for two different states of loading. The equations expressed in this point must be applied to these particles and between those loads.

4) The displacement gradient tensor is calculated using (44) and (46) to the contour particles using the two selected states of loading.

5) The deformation tensor is calculated using (48).

From a certain distance from the particle P, it is expected that the invariants of the deformation tensor will have not a great scattering in their values, assuring that exists a global tensor of behavior of the media.

Nowadays the application of the method is under development and in the near future is expected that the first numerical results will be obtained using the generated granular materials [3].

### 4.3 Stress formulation

In this point a proposal of formulation to obtain an equivalent stress tensor for a discrete particle model is presented.

As was stated in the previous point, a fictitious sphere is generated and a set of particles; inside, contour and exterior, are defined. Every effective contact is determined by a position vector $\overline{\boldsymbol{R}}$, referred to the global system of axis. The action of the exterior particle over the one belonging to the contour is exerted in the point where the effective contact takes place. In that contact exists a force $\bar{\mathcal{F}}$ and a torque $\bar{\mathcal{M}}$. Figure 7 shows a scheme of the position vector and the force and torque that occur in the effective contact.

The following conditions must be verified in order to fulfill the equilibrium:

$$\sum_{i=1}^{n} \bar{\mathcal{F}} = 0 \tag{51}$$

$$\sum_{i=1}^{n} (\bar{R} \wedge \bar{\mathcal{F}} + \bar{\mathcal{M}}) = 0 \tag{52}$$

The summation index i cover all the effective contacts belonging to the fictitious sphere.

In the other hand, a plane $\pi$ of normal $\bar{n}$ is defined. This plane cuts the fictitious sphere, dividing it in two halves:

- The outer half fulfills $\bar{R} \cdot \bar{n} > 0$
- The inner half fulfills $\bar{R} \cdot \bar{n} < 0$

The exterior particles exert two unitary actions, $\bar{\sigma}$ and $\bar{m}$, over the plane $\pi$. These unitary actions have the following expressions:

$$A \cdot \bar{\sigma} = \sum_{i=1}^{n} \bar{\mathcal{F}} \tag{53}$$

$$A \cdot \bar{m} = \sum_{i=1}^{n} (\bar{\mathcal{M}} + \bar{R} \wedge \bar{\mathcal{F}}) \tag{54}$$

The summation is extended to every effective contact of the fictitious sphere of center P and radius R, situated in the outer half and A is the area of the circle (A= $\pi \cdot R^2$).

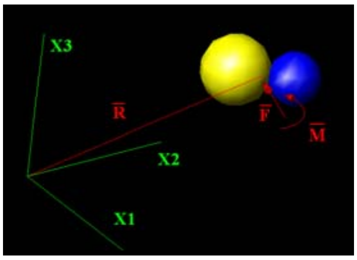


Figure 7.- Position vector and existing forces in an effective contact.

If the outer half of the fictitious sphere is considered as a continuous surface, a summation of forces and torques can be done. By doing this summation, an average stress is obtained acting over the plane $\pi$. In this way, if the stress tensor would exist, it will produce the following linear relation:

$$\sigma_i = T_{ij} n_j \tag{55}$$

Where; $T_{ij}$ is the Cauchy stress tensor; i is the index that indicates the orientation of the stress and j indicates de orientation of the plane where the stress is acting. That is to say, $T_{ij}$ is used as a transformation to obtain the component parallel to $X_i$ of the stress over the plane of normal $n_j$. $\sigma_{ij}$ is the tension acting over the plane $n_j$ in the direction of the axis $x_i$; and $n_j$ is the normal to the plane j.

If the enounced tension is extended to the whole set of particles of the contour, the average stress over a plane of certain orientation would be:

$$\sigma^k = \frac{(\sum \mathcal{F})}{\pi R^2} \tag{56}$$

Where: $\sigma^k$ is the average stress over a plane of normal $n^k$; $\mathcal{F}$ are the forces acting on the plane $n^k$; and R is the radius of the fictitious sphere.

The calculus of the stress tensor is done statistically as was done for the deformation tensor using the displacement gradient tensor. In order to do this the best adjustment to the stress tensor is searched, $\sigma^{k*}$.

To define the error function a stress $\sigma^k$ is calculated using (56) over a certain plane of orientation $n^k$. The searched stress tensor $T_{ij}$ will produce a theoretical stress $\sigma^{k*}$ over the same plane. Both values will differ producing an error. The quadratic error of both tensions is defined as follow:

$$\varepsilon_i{}^k = \sigma^{k*} - \sigma^k = T_{ij} n^k - \sigma^k \tag{58}$$

If the modulus of this error is raise to the second power, the average quadratic error is obtained for a certain plane $n^k$.

$$E^k = |\varepsilon^k|^2 = \sum_{i=1}^{3} \left(T_{ij} n^k - \sigma^k\right)^2 \tag{59}$$

The total quadratic error corresponding to "h" characteristic planes will be:

$$E = \sum_{k=1}^{h} E^k \quad = |\varepsilon^k|^2 = \sum_{k=1}^{h} \left(\sum_{i=1}^{3} \left(T_{ij} n^k - \sigma^k\right)^2\right) \tag{60}$$

To obtain the stress tensor, the error must be minimized:

$$\frac{dE_r}{dT_{ij}} = 0 \tag{61}$$

$$\frac{dE_r}{dT_{ij}} = 2\sum\left(T_{is}n_s^k - \sigma_i^k\right)n_j^k \tag{62}$$

$$T_{ij}\left(\sum_{k=1}^{13} n_s^k n_j^k\right) - \left(\sum_{k=1}^{13} \sigma_i^k n_j^k\right) = 0 \tag{63}$$

This equalty can be rewritten as:

$$T_{ij}\left(\sum_{k=1}^{h} n_s^k n_j^k\right) = \left(\sum_{k=1}^{h} \sigma_i^k n_j^k\right) \tag{64}$$

$$T_{is}A_{sj} = H_{ij} \tag{65}$$

Where;

$T_{is}$ is the equivalent stress tensor of the media.

$A_{sj} = \left(\sum_{k=1}^{h} n_s^k n_j^k\right)$ The k index covers the h planes, while s and j covers all the particles belonging to the contour.

$H_{ij} = \left(\sum_{k=1}^{h} \sigma_i^k n_j^k\right)$ The k index covers the h planes, while s and j covers all the particles belonging to the contour.

The unknown factor is $T_{ij}$ and it can be finally obtained:

$$T_{ij} = H_{is}A_{js}^{-1} \tag{66}$$

It is expected that from a certain distance from the particle P, the invariants of the stress tensor will not have a great scattering in their values, assuring that a global tensor of behavior of the media exists.

Nowadays the application of the method is under development and in the near future is expected that the first numerical results will be obtained using the generated granular materials [3].

Similarly to the formulation that has been written for the stress tensor, a formulation for the torque tensor can be enounced:

$$M_{ij} = H_{is}^M A_{js}^{-1M} \tag{67}$$

Where:

$M_{ij}$ is the torque tensor.

$H_{is}^M = \left(\sum_{k=1}^{h} m_i^k n_j^k\right)$ The k index covers the h planes, while s and j covers all the particles belonging to the contour.

$A_{js}^M = \left(\sum_{k=1}^{h} n_s^k n_j^k\right)$ The k index covers the h planes, while s and j covers all the particles belonging to the contour.

### 4.4 Quality of the adjustment

To obtain a measure of the quality of the adjustment, once the stress tensor has been calculated using (66), it can be inserted in the expression of the total quadratic error (60). In this way, a value of the average quadratic error for a given load will be calculated:

$$E = \sum_k \sum_i \left(\frac{\left(T_{ij}n^k - \sigma^k\right)^2}{\left(T_{ij}n^k\right)^2}\right) \tag{68}$$

But in our opinion is better to obtain an average value of the unitary error, being this error:

$$E_u = \frac{1}{k}\sum_k \sum_i \left(1 - \frac{\sigma^k}{T_{ij}n^k}\right)^2 \tag{69}$$

Where; k is the number of characteristic planes used for the calculi.

## 5 ENERGY FORMULATION

### 5.1 Initial ideas

In this point a formulation to study how the energy is given to the media by increasing the external load and how it is invested into the system by using the first principle of thermodynamics.

Using the macroelement of radios R and centered in P defined in previous points (as if it were a body), for the development of this formulation the particles belonging to the exterior (E set); the contour (C set) and the interior (I set) are used. Figure 8 shows a scheme of the variables that will be used from now on. These variables as can be seen in Figure 8 are:

- The contour particle K.

- The effective contact (as defined previously) $K_i$ that belongs to the particle K.
- $\mathcal{F}^{ki}$ is the force that is acting in the effective contact. This force is formed up by a normal and a shear force as has been stated in previous points.
- $\mathcal{M}^{ki}$ is the torque that is acting in the effective contact. This torque is formed up by a normal and a shear torque as was shown in Figure 1.
- $u^k$ are the displacements of the particle K that produce the forces $\mathcal{F}$.
- $\phi^k$ are the rotations of the particle K that generates the torques $\mathcal{M}$.

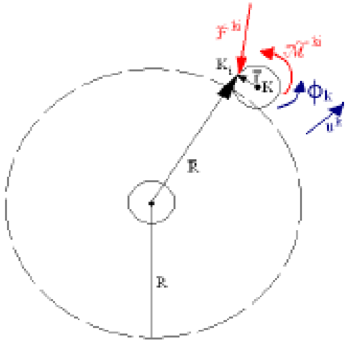


Figure 8.- Scheme of forces and displacements in an effective contact of a macroelement.

Applying the first principle of thermodynamics:

$$\dot{\mathcal{K}} + \dot{\mathcal{E}} = P^c + P^d + \dot{Q} \tag{70}$$

Where; $\dot{\mathcal{K}}$ is the material derivative of the kinetic energy respect time; $\dot{\mathcal{E}}$ is the material derivative of the internal energy respect time; $P^c$ is the potential energy of the contour forces ($\bar{\mathcal{F}}$ and $\bar{\mathcal{M}}$) belonging to the effective contacts (defined in previous points); $P^d$ is the potential energy of the volumetric forces; and $\dot{Q}$ is the velocity of supply of heat to the body.

Using D'Alambert´s principle can be said that:

$$\dot{\mathcal{K}} + P^c + P^d + P^i = 0 \tag{71}$$

Where; $P^i$ is the potential energy of the interior forces ($\bar{\mathcal{F}}$ and $\bar{\mathcal{M}}$) of the existing contacts of the interior particles with the contour particles of the macroelement.

Equaling (70) to (71), the resulting equation allows clearing the concept of internal energy:

$$\dot{\mathcal{E}} = Q - P^i \tag{72}$$

For the case of study, the energy consumption in the macroelement is admitted to be:
- $P^d = 0$ because there are not volumetric forces.
- $\dot{\mathcal{K}} = 0$ because the loading process is very slow and it can be considered almost static.

With these suppositions result that:

$$\dot{\mathcal{E}} = P^c + \dot{Q} \tag{73}$$

$$P^c = -P^i \tag{74}$$

## 5.2 The discrete media

As has been said in the previous point, two different potential energies associated to two set of particles must be studied; the potential energy of the contour forces; and the potential energy of the inside forces.

A) Potential energy of the contour forces

For a certain particle K that belongs to the contour set (C set) and has an effective contact $K_i$, the potential energy for that particle is called $P^{ck}$. This potential has the expression:

$$P^{ck} = \sum_i \left[\bar{\mathcal{F}}^{ki} \cdot \left(\dot{\bar{u}}^k + \dot{\bar{\phi}}^k \wedge \bar{r}^k\right) + \bar{\mathcal{M}}^{ki} \cdot \dot{\bar{\phi}}^k\right] = \left(\sum_i \bar{\mathcal{F}}^{ki}\right) \cdot \dot{\bar{u}}^k + \left[\sum_i (\bar{\mathcal{M}}^{ki} + \bar{\mathcal{F}}^{ki} \wedge \bar{r}^k)\right] \cdot \dot{\bar{\phi}}^k \tag{75}$$

The total potential energy for the whole set of particles of the contour with effective contacts will be:

$$P^c = \sum_k P^{ck} \tag{76}$$

The summation of $k$ is extended to the particles K of the contour. In the other hand, the total potential energy can be factorized as:

$$P^c = P^{cu} + P^{c\phi} \tag{77}$$

$$P^{cu} = \sum_k (\sum_i \bar{\mathcal{F}}^{ki}) \cdot \dot{\bar{u}}^k \tag{78}$$

$$P^{c\phi} = \sum_k (\sum_i (\bar{\mathcal{M}}^{ki} + \bar{r}^k \wedge \bar{\mathcal{F}}^{ki})) \cdot \dot{\bar{\phi}}^k \tag{79}$$

B) Potential energy of the inside forces

From the first principle of thermodynamics has been obtained (74) but it can be deduced directly saying that the effect of the potential energy of the inside forces ($P^i$) can be expressed:

$$P^i = P^{ii} + P^{ic} \tag{80}$$

Where; $P^{ii}$ is the potential energy of all the contacts that belongs to a particle of the inside set and are not in contact with a particle of the contour set; $P^{ic}$ is the potential energy of all the contacts that belongs to a particle of the inside set and are in contact with a particle of the contour set.

For a certain contact between two particles (1 and 2) and using the action-reaction law, it is known that in that contact:

$$\bar{\mathcal{F}}^1 + \bar{\mathcal{F}}^2 = 0 \tag{81}$$

$$\bar{\mathcal{M}}^1 + \bar{\mathcal{M}}^2 = 0 \tag{82}$$

$$P^{ii} = \sum_k \left[\sum_i (\bar{\mathcal{F}}^{ki}) \cdot \dot{\bar{u}}^k + \sum_i (\bar{\mathcal{M}}^{ki} + \bar{r}^k \wedge \bar{\mathcal{F}}^{ki}) \dot{\bar{\phi}}^k\right] \tag{83}$$

The inside particles are all in equilibrium, that is to say:

$$\sum_i \bar{\mathcal{F}}^{ki} = 0 \tag{84}$$

$$\sum_i (\bar{\mathcal{M}}^{ki} + \bar{r}^k \wedge \bar{\mathcal{F}}^{ki}) = 0 \tag{85}$$

So it can be said that:

$$P^{ii} = 0 \tag{86}$$

Analogous at has been done for the inside particles, for the particles that belongs to the $P^{ic}$ set can be expressed the potential energy of the inside effective contacts as:

$$P^{ic} + P^c = 0 \tag{87}$$

$$P^{ic} = -P^c \tag{88}$$

$$P^i = P^{ic} = -P^c \quad \text{<C.Q.D.>} \tag{89}$$

### 5.3 The continuous media

In this point, the media will be considered as a continuous media and will be used the formulation proposed in the previous points.

In the macroelement of radious R (body B) that was defined, we were able to calculate as has been stated in previous points of this paper, the following:

- The tensors T and M in the field of stresses.
- The tensors F and K in the field of deformations.
- The displacements $u$ and the rotations $\phi$.

Both the potential energy of the contour forces and the potential energy of the inside forces will be studied as was done in point 5.3.

The potential energy of the contour forces, $P^c$ is expressed:

$$P^c = \int_{dB} (\dot{u} \cdot \sigma + \dot{\phi} \cdot m) da = \int_{dB} [\dot{u} \cdot (T \cdot n) + \dot{\phi} \cdot (M \cdot n)] da = \int_{dB} (\dot{u} \cdot T + \dot{\phi} \cdot M) \cdot n \, da \tag{90}$$

Using the Gauss-Ostrogradsky theorem (Divergence theorem) (90) can be rewritten:

$$P^c = \int_B [T : \nabla\dot{u} + M : \nabla\dot{\phi}] dV + \int_B [(T\nabla)\dot{u} + (M\nabla)\dot{\phi}] dV \tag{91}$$

$$P^c = \int_B [T : (\nabla\dot{u} + \varepsilon\dot{\phi}) + M : \nabla\dot{\phi}] dV + \int_B [(T\nabla)\dot{u} + (M\nabla - \varepsilon\mathrm{T})\dot{\phi}] dV \tag{92}$$

Considering that do not exist volumetric forces inside the body B (macroelement) the equilibrium equations of Cosserat´s media will be:

$$T\nabla = 0 \qquad and \qquad M\nabla - \varepsilon T = 0 \tag{93}$$

Substituting in (92) it is finally obtained that:

$$P^c = \int_B [T : (\nabla\dot{u} + \varepsilon\dot{\phi}) + M : \nabla\dot{\phi}] dV = \frac{4\pi R^3}{3} [T : (\nabla\dot{u} + \varepsilon\dot{\phi}) + M : \nabla\dot{\phi}] \tag{94}$$

In Cosserat´s medias is fundamental the relative stretch tensor, *e*:

$$e = F - R^c \tag{95}$$

Where; $R^c$ is $R^c = \exp(-\varepsilon\phi)$, considering that the deformation is a finite deformation.

If the deformation is considered to be small it can be approximated by; $R^c = I - \varepsilon\phi$.

After this it can be formulated that:

$$e = F - I + \varepsilon\phi = \nabla u + \varepsilon\phi \tag{95}$$

In addition:

$$K = \nabla\phi \tag{96}$$

Taking into account this tensor *e* and the tensor *K* that was defined in (46), $P^c$ can be rewritten as:

$$P^c = \frac{4\pi R^3}{3}\left(T:\dot{e} + M:\dot{K}\right) \tag{98}$$

Considering the expression (89) the potential of the inside forces can be written as:

$$P^i = -\frac{4\pi R^3}{3}\left(T:\dot{e} + M:\dot{K}\right) \tag{99}$$

### 5.4 Results adjustments

As was stated previously and using (77), (89) and (99) the following expression relates the potential energy of the inside forces of the continuous media to the potential of the contour forces of the discrete media:

$$\frac{4\pi R^3}{3}\left[T:\dot{e} + M:\dot{K}\right] = \sum_k \left[\sum_i(\bar{\mathcal{F}}^{ki}) \cdot \dot{\bar{u}}^k + \sum_i(\bar{\mathcal{M}}^{ki} + \bar{r}^k \wedge \bar{\mathcal{F}}^{ki})\dot{\bar{\phi}}^k\right] \tag{100}$$

Both members of (100) can be calculated separately and independently by considering the media first as a continuous media and then as a discrete particle media. By doing this calculus and comparing the results obtained from the continuous point of view and from the discrete approach an adjustment of the statistic values of the average tensors T, e, M and K can be done. Defining a parameter, $\lambda^2$, to represent the quality of the adjustment:

$$\lambda^2 = \frac{P^c}{P^i} = \frac{3}{4\pi R^3}\frac{\sum_k\left[\sum_i(\bar{\mathcal{F}}^{ki})\cdot\dot{\bar{u}}^k + \sum_i(\bar{\mathcal{M}}^{ki} + \bar{r}^k\wedge\bar{\mathcal{F}}^{ki})\dot{\bar{\phi}}^k\right]}{[T:\dot{e}+M:\dot{K}]} \tag{101}$$

The tensors can be rewritten as follow:

$$T^* = \lambda \cdot T \qquad M^* = \lambda \cdot M \qquad \dot{e}^* = \lambda \cdot \dot{e} \qquad K^* = \lambda \cdot K \tag{102}$$

Another possibility to adjust the result would be to establish two different correction factors, $\lambda_u$ and $\lambda_\Phi$, depending on if the correction is done in the field of movements or in the field of rotations, respectively.

### 5.5 Analysis of the work

The program that has been developed loads a discrete particle media with a certain load $\mathcal{L}$, that can be; an isotropic compression; an oedometric load; etc… This load cannot be applied directly. The load must be applied iteratively and in defined increments. This incremental loading process allows identifying which contacts develop plastic movements and which not.

It can be assumed that the load is a time function. If the loading steps would be of the same quantity it could be possible to establish a relation between the load and the time. Being:

$$\dot{\mathcal{L}} = \frac{d\mathcal{L}}{dt} \tag{102}$$

$$\mathcal{L} = \int_0^t \dot{\mathcal{L}}\, dt = \int_0^t d\mathcal{L} = \sum \Delta\mathcal{L} \tag{104}$$

Where the integral is related to the continuous loading in time and the summation is related to the incremental loading process.

To obtain the work done by the contour particles using the potential energy of the C set particles ($P^c$) is used the expression (77). This allows us to analyze the work done due to the displacement and the rotation of a particle of the media.

In the plane of contact, $K_i$ (contour particle K and effective contact *i* belonging to that particle) the increment of internal work $\Delta W$ due to the increment of external load $\Delta\mathcal{L}$ is the addition of every partial increment of the work done by the components $\Delta W_u$ and $\Delta W_\phi$. These increments are produced by the forces $\mathcal{F}$ and by the torques $\mathcal{M}$ acting over the particle K and in the contact $i$ after having moved $(du)$ and rotate $(d\phi)$ by effect of the external load. Translating this into mathematical language:

$$\Delta W = \Delta W_u + \Delta W_\phi \tag{105}$$

$$\Delta W_{uFN} = \mathcal{F}_N \cdot du \tag{106}$$

$$\Delta W_{uFT} = \mathcal{F}_T \cdot du \tag{107}$$

$$\Delta W_{\phi MF} = (r \wedge \mathcal{F}_T + \mathcal{M}_F) \cdot d\phi \tag{108}$$

$$\Delta W_{\phi MT} = \mathcal{M}_T \cdot d\phi \tag{109}$$

Knowing that:

$$r \wedge \mathcal{F}_N = 0 \quad (110)$$

These distinctive components of the work can be plastic or elastic. The following hypotheses have been done in the model and impact on the different values of the components of the work that had been defined:

- The component $\Delta W_{uFN}$ is always elastic, because the law of behavior that defines the normal force is Hertz's Law (1) which is an elastic law although it is a non-linear law. In future improvements of the model this restriction will be deleted.

- The other three components of the work ($\Delta W_{uFT}$, $\Delta W_{\phi MF}$ and $\Delta W_{\phi MF}$) elastic or plastic depending on if the values of $\mathcal{F}_T$, $\mathcal{M}_F$ and $\mathcal{M}_T$ have reached the limit conditions expressed in (3) and (10) to (15), respectively, or not.

Finally, the total work done by the system can be decomposed into an elastic work and a plastic work. Expressing this:

$$\Delta W = \Delta W^E + \Delta W^P \quad (111)$$

The total work, $\Delta W^T$ can be written as:

$$\Delta W^T = \Delta W_u^E + \Delta W_\phi^E + \Delta W_u^P + \Delta W_\phi^P \quad (112)$$

## 6 CONCLUSIONS

This paper presents a proposal of formulation to calculate the stress, torque, deformation and curvature tensor for discrete particle medias, welded or non-welded, in order to study them as if they were continuous.

The appliance of this formulation is conditioned to that the output variables from the discrete particle model are: displacements and rotations of the particles in addition to forces and torques in every existing contact.

The enounced equations use classical mechanical concepts and statistical criteria for minimum squared adjustments.

With this methodology the knowledge acquired from the mechanical variables of a discrete particle model (forces, torques, displacements and rotations) can be changed into continuous mechanical concepts (stress, deformations and curvatures) creating a statistical mechanic of the discrete particle models.

This mechanic contribute to create a theory to facilitate future developments related to internal analysis of granular and particle medias, such as pyroclastic rocks, macroporous rocks and coarse granular materials.

In addition to the mechanical concepts a different approach is presented using the first thermodynamic principle. The statistical average tensor are adjusted with a different process as was enounced using the mechanical point of view.

## 7 REFERENCES

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